U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

2010 INCITE Projects

at the Argonne Leadership Computing Facility

Astrophysics

Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models
Donald Lamb, The University of Chicago
Intrepid Allocation: 70,000,000 hours

Biological Sciences

Computational Protein Structure Prediction and Protein Design
David Baker, University of Washington
Intrepid Allocation: 50,000,000 hours

Protein-Ligand Interaction Simulations and Analysis
T. Andrew Binkowski, Argonne National Laboratory
Intrepid Allocation: 25,000,000 hours

Millisecond Molecular Dynamics of Chaperoning of Unfolded Polypeptide Chains by HSP70
Harold Scheraga, Cornell University
Intrepid Allocation: 6,000,000 hours

Simulation and Modeling of Membrane Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions
Igor Tsigelny, University of California—San Diego
Intrepid Allocation: 5,000,000 hours

Chemistry

High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels
Jacqueline Chen, Sandia National Laboratories
Intrepid Allocation: 2,000,000 hours

Molecular Simulation of Complex Chemical Systems
Christopher Mundy, Pacific Northwest National Laboratory
Intrepid Allocation: 2,000,000 hours

Large Eddy Simulation of Two-Phase Flow Combustion in Gas Turbines
Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Intrepid Allocation: 8,000,000 hours

Prediction of Bulk Properties Using High-Accuracy *Ab Initio* Methods Interfaced with Dynamical Calculations
Theresa Windus, Ames Laboratory
Intrepid Allocation: 8,000,000 hours

Computer Science

Scalable System Software for Performance and Productivity
Ewing Lusk, Argonne National Laboratory
Intrepid Allocation: 5,000,000 hours

BG/P Plan 9 Measurements on Large-Scale Systems
Ronald Minnich, Sandia National Laboratories
Intrepid Allocation: 1,000,000 hours

Performance Evaluation and Analysis Consortium End Station
Patrick H. Worley, Oak Ridge National Laboratory
Intrepid Allocation: 8,000,000 hours

Earth Science

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz
Thomas Jordan, Southern California Earthquake Center
Intrepid Allocation: 7,000,000 hours

Climate-Science Computational End Station Development and Grand Challenge Team
Warren Washington, National Center for Atmospheric Research
Intrepid Allocation: 30,000,000 hours

Energy Technologies

Advanced Reactor Thermal Hydraulic Modeling
Paul Fischer, Argonne National Laboratory
Intrepid Allocation: 30,000,000 hours

Predictions of Thermal Striping in Sodium-Cooled Reactors
Andrew Siegel, Argonne National Laboratory
Intrepid Allocation: 10,000,000 hours

Argonne NATIONAL LABORATORY

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2010 INCITE Projects

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Energy Technologies (cont.)

High-Resolution Global Simulation of Plasma Microturbulence
William Tang, Princeton Plasma Physics Laboratory
Intrepid Allocation: 12,000,000 hours

Petascale Particle-In-Cell Simulations of Fast Ignition
John Tonge, University of California—Los Angeles
Intrepid Allocation: 7,000,000 hours

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air
Jack Wells, Oak Ridge National Laboratory
Intrepid Allocation: 12,000,000 hours

Engineering

Petascale Adaptive Computational Fluid Dynamics for Applications with High Anisotropy
Kenneth Jansen, Rensselaer Polytechnic Institute
Intrepid Allocation: 10,000,000 hours

Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence
Susan Kurien, Los Alamos National Laboratory
Intrepid Allocation: 25,000,000 hours

Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability
Sanjiva Lele, Stanford University
Intrepid Allocation: 12,000,000 hours

Simulation of "High" Reynolds Number Turbulent Boundary Layers
Robert Moser, University of Texas at Austin
Intrepid Allocation: 33,000,000 hours

Overcoming the Turbulent-Mixing Characterization Barrier to Green Energy and Propulsion Systems
Anurag Gupta, GE Global Research
Intrepid Allocation: 19,000,000 hours

Materials Science

Quantum Simulations of Nanostructured Materials for Renewable Energy Applications
Giulia Galli, University of California—Davis
Intrepid Allocation: 1,000,000 hours

Modeling the Rheological Properties of Concrete
William George, National Institute of Standards and Technology
Intrepid Allocation: 2,000,000 hours

Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
Jeffrey Greeley, Argonne National Laboratory
Intrepid Allocation: 10,000,000 hours

Electronic Structure Calculations of Nano Solar Cells
Lin-Wang Wang, Lawrence Berkeley National Laboratory
Intrepid Allocation: 1,000,000 hours

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles
Christopher Wolverton, Northwestern University
Intrepid Allocation: 8,000,000 hours

Physics

Unbalanced Magnetohydrodynamic Turbulence
Stanislav Boldyrev, University of Wisconsin—Madison
Intrepid Allocation: 25,000,000 hours

Research into the Systematics of Type Ia Supernovae
Alan Calder, Stony Brook University
Intrepid Allocation: 35,000,000 hours

Large-Scale Condensed Matter and Fluid Dynamics Simulations
Peter Coveney, University College London
Intrepid Allocation: 40,000,000 hours

Computational Nuclear Structure
David Dean, Oak Ridge National Laboratory
Intrepid Allocation: 15,000,000 hours

Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond
Denise Hinkel, Lawrence Livermore National Laboratory
Intrepid Allocation: 45,000,000 hours

Lattice QCD
Paul Mackenzie, Fermilab
Intrepid Allocation: 67,000,000 hours

Allocations are in core-hours on Intrepid, a 557 TF Blue Gene/P system.

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